Benzene, 1-ethyl-3-(1-methylpropyl)

Other names: 1-Ethyl-3-s-Butylbenzene
Inchi: InChI=1S/C12H18/c1-4-10(3)12-8-6-7-11(5-2)9-12/h6-10H,4-5H2,1-3H3
InchiKey: KTCNWORLNAKRDZ-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCc1cccc(C(C)CC)c1
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	150.50	kJ/mol	Joback Method
hf	-71.23	kJ/mol	Joback Method
hfus	16.96	kJ/mol	Joback Method
hvap	44.86	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.763		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1170.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1366.60		NIST Webbook
ripol	1366.60		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1367.00		NIST Webbook
tb	505.18	K	Joback Method
tc	710.08	K	Joback Method
tf	248.94	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.40	J/mol×K	505.18	Joback Method
cpg	363.34	J/mol×K	539.33	Joback Method

cpg	379.40	J/mol×K	573.48	Joback Method
cpg	394.59	J/mol×K	607.63	Joback Method
cpg	408.95	J/mol×K	641.78	Joback Method
cpg	422.51	J/mol×K	675.93	Joback Method
cpg	435.30	J/mol×K	710.08	Joback Method
dvisc	0.0037035	Pa×s	248.94	Joback Method
dvisc	0.0015687	Pa×s	291.65	Joback Method
dvisc	0.0008275	Pa×s	334.35	Joback Method
dvisc	0.0005046	Pa×s	377.06	Joback Method
dvisc	0.0003403	Pa×s	419.77	Joback Method
dvisc	0.0002468	Pa×s	462.47	Joback Method
dvisc	0.0001890	Pa×s	505.18	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R52840&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume